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1. GENERAL INFORMATION

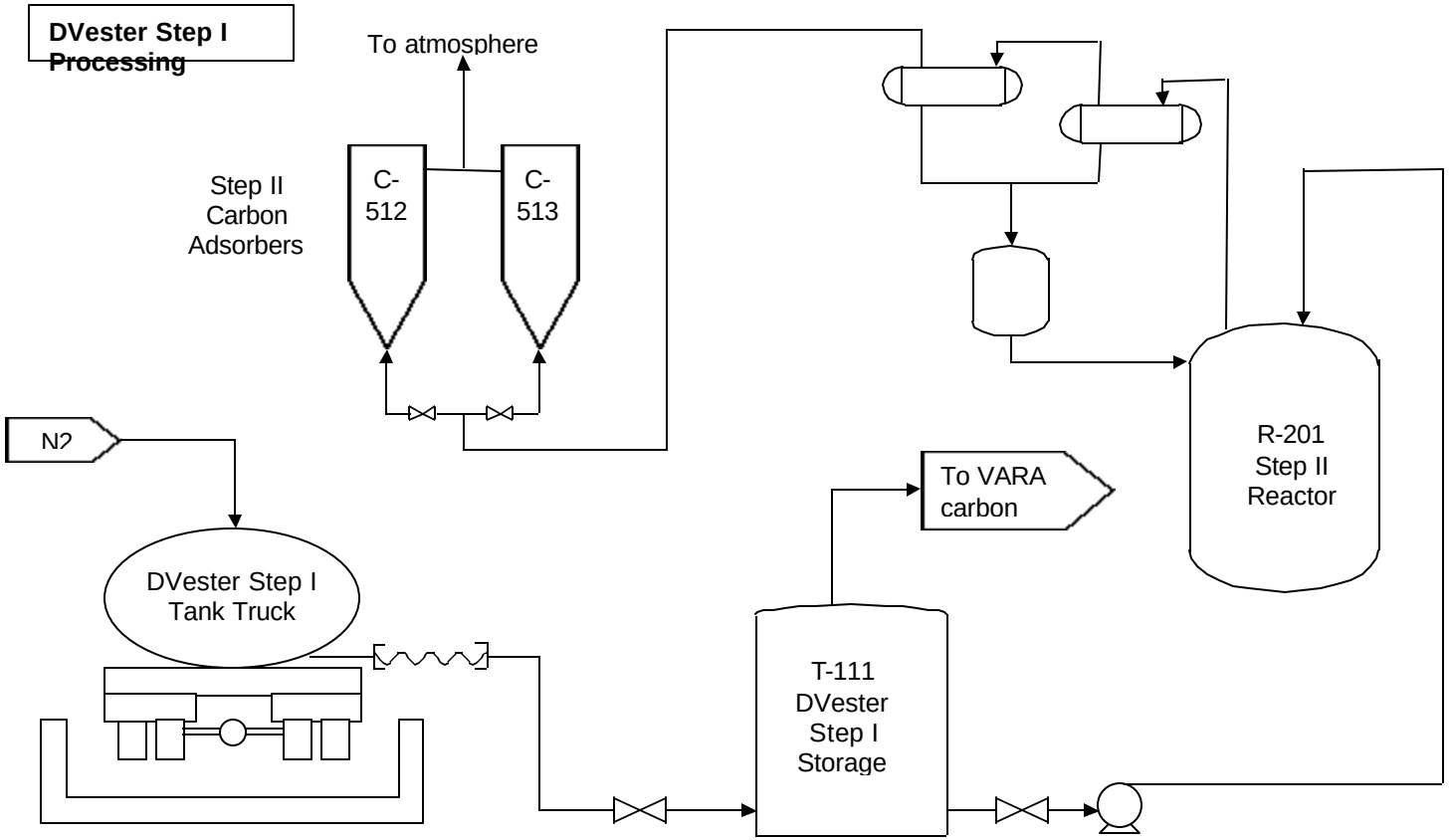
1.1. CAS NUMBER 63721-05-1

1.2. CHEMICAL NAME Methyl 3,3-dimethyl-4, pentenoate

1.3. EXPOSURE (CLOSED SYSTEM)

1.3.1. NUMBER OF SITES Until 2002, methyl 3,3-dimethyl-4-pentenoate was only manufactured at FMC's Baltimore site. This site no longer has the capability to produce this chemical and relies solely on an offshore producer as the source. FMC's Baltimore location is the only site processing methyl 3,3-dimethyl-4-pentenoate.

1.3.2. PROCESS DESCRIPTION: DVester Step I (methyl dimethyl pentenoate) is unloaded from tank trucks to T-111 using low pressure nitrogen. T-111 vents to the water scrubbers and then to the VARA carbon adsorption system. The Step I is charged to the R-201 reactor, where it reacts with carbon tetrachloride to form DVester Step II. The step II reaction system vents to C-512 and C-513, the step II carbon adsorbers. The step II product is then transferred to one of two storage tanks. The entire system is closed.



1.3.3. MONITORING DATA:

Wastewater monitoring - Wastewater samples are taken before every pump down to the south plant carbon beds. The limit for Step I in the water is 450 ppm maximum. In 2002, our average concentration of Step I in this wastewater stream was 1.55 ppm.

IH Data – IH monitoring was conducted in 1987. Of twenty sample locations measured, only two locations detected the presence of Step I in the air. The FMC and OSHA guidelines for measurable quantities at the time were 10 ppm. The two readings were 1.0 ppm and 0.8 ppm with a limit of detection at the time of monitoring of 0.5 ppm.

1.3.4. PRESENCE IN DISTRIBUTED PRODUCT:

No DVEster Step I is present in the DVEster Finished Goods products.

1.3.5. TRANSPORT DATA:

Since 2002, FMC has relied solely on an offshore producer as the source of methyl 3,3-dimethyl-4-pentenoate. Methyl 3,3-dimethyl-4-pentenoate is delivered to the Baltimore site in tank trailers, directly off loaded into storage and then consumed. There is no additional transport of this chemical on site or off site.

Previously, Step I DVEster was packaged and transported to Syngenta (formerly ICI and Zeneca) in England for use in TFPAcid manufacture. This practice was ceased in 2002.

1.3.6. PRESENCE IN END USE PRODUCTS:

Methyl 3,3-dimethyl-4-pentenoate is reacted to greater than 99% conversion in the Step 2 DV Ester process. Residual methyl 3,3-dimethyl-4-pentenoate is removed with waste streams. This chemical is not included on Confidential Statements of Formula for end use products, including Permethrin Technical (279-3013).

Literature Search - Results from a Chemical Abstracts On-line Database literature search indicate that DVEster Step I is not present in other end-products.

2. PHYSICAL AND CHEMICAL DATA

2.1. MELTING POINT

No data available.

2.2. BOILING POINT

2.2.1 SOURCE #1

Test Substance: Methyl 3,3-dimethyl-4-pentenoate

Method: Unknown

GLP: No

Year:	1978
Results:	73 ° C @ 6.7 Kpa (50 mm Hg)
Data Quality:	4e
References:	“Permethrin Compendium”, M. Fishman, November 17, 1980

2.2.2. SOURCE #2

Test Substance:	Methyl 3,3-dimethyl-4-pentenoate
Method:	Vacuum distillation
GLP:	No
Year:	1983
Results:	95-99 ° C @ 140 mm Hg and 70 ° C @ 60 mm Hg
Data Quality:	4e
References:	United States Patent 4,374,264

2.3. VAPOR PRESSURE

Test Substance:	Methyl 3,3-dimethyl-4-pentenoate
Method:	Unknown
GLP:	No
Year:	Unknown
Results:	50 mm Hg@ 73°C
Data Quality:	4e
References:	FMC MSDS

2.4. PARTITION COEFFICIENT No data available.

2.5. WATER SOLUBILITY No data available.

3. ENVIRONMENTAL FATE AND PATHWAY

3.1. PHOTODEGRADATION

Test Substance:	Methyl 3,3-dimethyl-4, pentenoate
Method:	Estimated by the AOP program (v. 1.90) which estimates rate constants and half-lives of atmospheric reactions of organic compounds with hydroxyl radicals and ozone in the atmosphere.
GLP:	No
Year:	2000
Results:	For reaction with hydroxyl radicals, the predicted half-life is 4.7 hours with a rate constant of 2.72×10^{-13} cm^3/molecule-sec.
Remarks:	The photodegradation calculation by an acceptable method is assigned a reliability code of 2f.
References:	AOPWIN version 1.90, Syracuse Research Corporation, Syracuse, NY

3.2. STABILITY IN WATER (HYDROLYSIS)

Test Substance:	Methyl 3,3-dimethyl-4, pentenoate
Method:	Estimated by HYDROWIN program (v. 1.67)
GLP:	No
Year:	2000
Results:	The estimated half-life for this substance is 5.4 years at pH 8 and 54 years at pH 7.
Remarks:	The hydrolysis calculation by an acceptable method is assigned a reliability code of 2f.
References:	HYDROWIN version 1.67, Syracuse Research Corporation, Syracuse, NY

3.3. TRANSPORT/DISTRIBUTION (FUGACITY MODEL)

Test Substance:	Methyl 3,3-dimethyl-4, pentenoate
Method:	Estimated by EPI Suite program (v. 3.05)

GLP: No

Year: 2002

Results: Distribution using Level III Fugacity model

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.86	8.9	1000
Water	34.9	360	1000
Soil	62.1	360	1000
Sediment	0.206	1.44e+003	0

Remarks: The fugacity calculation by an acceptable method is assigned a reliability code of 2f.

References: EPI Suite version 3.05, Syracuse Research Corporation, Syracuse NY

3.4. BIODEGRADATION No data available.

4. ECOTOXICOLOGY

4.1. ACUTE TOXICITY TO FISH

Test Substance: Methyl 3,3-dimethyl-4-pentenoate

Method: EPA, 1975, Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. Ecological Research Series EPA-660/3-75-009. 61 p.

Test was conducted under static condition in 19 L uncovered jars which contained 15 L of natural, filtered (5 micrometers) sea water. Salinity was 29 parts per thousand. Temperature was maintained at 20°C +/- 1. Initial pH was 8 +/- 0.5 for all test concentrations and controls. The sheepshead minnows measured 7- 12 mm standard length. Mortality was < 3% during a 7-day acclimation period. The fish appeared to be in excellent condition at initiation of the test. Each test jar contained 10 fish. There was no aeration.

Sheepshead minnows were exposed to concentrations up to 100 ppm. Test material was dissolved in reagent grade acetone and pipetted into sea water in the appropriate test containers to obtain the desired concentrations. A vehicle control was run with a volume of acetone equal to that added to the highest test concentration.

Species: Sheepshead minnow (*Cyprinodon variegates)*

Test Concentration (nominal):	Less than or equal to 100 ppm
Exposure Period:	96 hours
Analytical Monitoring:	No
GLP:	No
Year:	1976
Results:	Sheepshead minnows were not apparently affected after 96 hours of exposure to methyl 3,3-dimethyl-4-pentenoate at concentrations less than or equal to 100 ppm. Dissolved oxygen remained >65% of saturation in all test concentrations and controls for the duration of the test. The final pH was 8 +/- 0.5 for all test concentrations and controls.
Conclusion:	The 96-hr LC_{50} was > 100 ppm.
Data Quality:	2d
References:	Acute Toxicity of four compounds to Sheepshead Minnows (*Cyprinodon variegates)*, EG&G, Bionomics, Study Number ACT 015.11-01, April 1976.

4.2. ACUTE TOXICITY TO AQUATIC INVERTEBRATES

No data available.

4.3. TOXICITY TO AQUATIC PLANTS

No data available.

5. TOXICITY

5.1. ACUTE TOXICITY

5.1.1. ORAL

Test Substance:	Methyl 3,3-dimethyl-4-pentenoate, >98% purity
Method:	US EPA Pesticide Assessment Guidelines; Subdivision F, Hazard Evaluation: Human and Domestic Animals, November, 1982; 81-1 Acute Oral Toxicity Study
Species/strain:	Sprague-Dawley

Sex:	Male and Female
No. Animals/Group:	5/sex/group
Dose:	6000, 5000, 4000 mg/kg
Post-dosing observation period:	14 days
GLP:	Yes
Year:	1984
Results:	Predominant clinical signs included decreased locomotion, recumbency, abdominogenital staining, ataxia and lacrimation. All signs subsided by day six of the study. All surviving animals gained weight by day 14 of the study. Survivors appeared normal at gross necropsy; findings among decedents included hemorrhagic lungs and intestines and blood in the intestines.
Conclusion:	The test material is classified as practically non-toxic with a LD50 for males of greater than 5000 mg/kg and the LD50 for females of 5498 mg/kg.
Data Quality:	1
References:	Acute Oral Toxicity of FMC 30098 Technical in Rats, FMC Study Number A1984-1541, October 15, 1985.

5.1.2. DERMAL

Test Substance:	Methyl 3,3-dimethyl-4-pentenoate, >98% purity
Method:	The test substance was applied topically to the backs of 10 rabbits, 5 rabbits per dosage, under occluded conditions for 24 hours. Observations for toxicity were conducted daily, irritation was evaluated after 1, 2, 3, 4, 7 and 14 days.
Species/strain:	New Zealand White Rabbits
No. Animals:	5 animals/group
Dose:	300 mg/kg and 20.0 mg/kg
Vehicle:	None
Exposure Period:	24 hours

Post-exposure observations:	Observations for toxicity: daily Observations for irritation: 1, 2, 3, 4 and 7 days
GLP:	Yes
Year:	1985
Results:	All of the animals survived the 14-day observation period. No signs of intoxication were observed. Slight erythema was observed in both groups during the first 48 hours. Within 72 hours, all irritation had resolved. However, four days after dosing, redness reappeared on four animals in the 300 mg/kg group and persisted to day 7. Additionally, one animal exhibited desquamation on day 7. At termination, day 14, slight redness persisted on two animals. No unusual findings were observed at gross necropsy.
Conclusion:	The test substance was practically non-toxic and minimally irritating.
Data Quality:	2c
References:	Preliminary Dermal Toxicity/Irritation of FMC 30098 Technical in Rabbits, FMC Toxicology Laboratory, FMC Study A84-1485, October 128, 1985.

5.1.3. INHALATION

Test Substance:	Methyl 3,3-dimethyl-4-pentenoate, >98% purity
Method:	A group of five male and five female Sprague-Dawley rats was exposed to the vapor of the test substance for six hours at an analytically determined concentration of 2000 ppm. Observations for toxicity and mortality were performed frequently during the exposure, on removal of the rats from the chamber, at one hour post-exposure, twice daily for 13 days and once on day 14. Individual body weights were recorded immediately prior to exposure (day 0) and on days 7 and 14. On day 14 all animals were sacrificed and gross necropsy examinations were performed. A similar group of control rat, sham-exposed to room air only, was also included in the study.
Species/strain:	Sprague-Dawley
No. Animals:	5/sex/group
Dose:	2000 ppm
Vehicle:	undiluted
Exposure Period:	6 hours
Post-exposure	

observation period:	14 days
GLP:	Yes
Year:	1987
Results:	There were no deaths during the study. Clinical signs noted among test rats during and shortly after exposure included squinting eyes, labored breathing patterns, decreased motor activity, decreased responsiveness and uncoordinated movements. On removal from the chamber and one-hour post dose, all of the exposed animals exhibited uncoordinated gait. One female exhibited red material around the right eye upon removal from the chamber and one male exhibited chromodacryorrhea on Day 1. All of the exposed rats appeared otherwise normal from Days 1 to 14. The only abnormal signs noted in control rats during the study were sporadic incidents of lacrimation and red material around the eye noted during and soon after exposure. All signs subsided by study Day 2. Body weight gains were similar between control and test animals. Renal pelvis dilation of the kidneys was found in one male in the control group and one male from the test material exposed group. These findings are considered to be developmental variations commonly found in this strain of rat and are not considered to be related to treatment. No gross lesions were observed in any of the remaining animals. A six-hour exposure of rats to an analytically determined concentration of 200 ppm produced no mortality, body weight changes or gross necropsy findings. The clinical signs observed are suggestive of both slight inhibition and depression of the central nervous system as a possible toxic response to the vapors. Recovery was rapid and no lasting effects were observed.
Conclusion:	The inhalation LC_{50} of the test substance was greater than 2000 ppm.
Data Quality:	2c
References:	Acute Inhalation Toxicity Screen of FMC 39008 in Rats, FMC Toxicology Laboratory, FMC Study A85-1652, May 13, 1987.

5.2. REPEATED DOSE TOXICITY No data available.

5.3. GENETIC TOXICITY IN VITRO AND IN VIVO

5.3.1. GENE MUTATION

Test Substance:	Methyl 3,3-dimethyl-4-pentenoate, >98% purity
Method:	*Salmonella typhimurium*/Mammalian Microsome Plate Incorporation Mutagenicity Assay (Ames Test). The test was conducted using *Salmonella typhimurium* tester strains TA1535, TA1537, TA1538, TA98, TA100 with and without metabolic activation by rat liver microsomes, S9, using the standard protocol. Appropriate positive and negative controls were included in the assay. The positive controls included

sodium azide, 9-aminoacridine, 2-nitrofluorene and 2-anthramine. The negative control was the solvent DMSO. The criteria for positive results were derived from Principles of Genetic Toxicology (1980).

The test article was solubilized in DMSO and serially diluted immediately before its use in the mutagenicity assay. Five doses of the test material were plated with all five tester strains with and without metabolic activation. All solvent controls and test article doses were plated in triplicate.

Type:	*In vitro* mutagenicity in bacteria
System of Testing:	*Salmonella typhimurium* TA1535, TA1537, TA1538, TA98, TA100 with and without metabolic activation by Aroclor induced rat liver microsomes, S9.
Concentration:	100 to 10,000 ug/plate
Metabolic Activation:	S9
GLP:	Yes
Year:	1986
Results:	The test material did not cause a positive response in any of the five tester strains with or without metabolic activation.
Conclusion:	The test substance was not mutagenic with or without metabolic activation.
Data Quality:	2d
References:	Salmonella/Mammalian-Microsome Plate Incoproration Mutagenicity Assy (Ames Test), FMC Genetic Toxicology Laboratory, FMC Study Number A84-1450.

Brusick, D. Principles of Genetic Toxicology. P. 195, Plenum Press, New York, 1980.

5.3.2. CHROMOSOMAL ABERRATION No data available.

5.4. REPRODUCTIVE TOXICITY No data available.

5.5. DEVELOPMENTAL TOXICITY/ TERATOGENICITY No data available.

CRITERIA FOR RELIABILITY CODES
(Adapted from Klimisch et al 1997)

Code of Reliability	Category or reliability
1	**Reliable without restriction**
1a	GLP guideline study (OECD, EC, EPA, FDA, etc.)
1b	Comparable to guideline study
1c	Test procedure in accordance with generally accepted scientific standards and described in sufficient detail
2	**Reliable with restrictions**
2a	Guideline study without detailed documentation
2b	Guideline study with acceptable restrictions
2c	Comparable to guideline study with acceptable restrictions
2d	Test procedure in accordance with national standard methods with acceptable restrictions
2e	Study well documented, meets generally accepted scientific principles, acceptable for assessment
2f	Accepted calculation method
2g	Data from handbook or collection of data
3	**Not reliable**
3a	Documentation insufficient for assessment
3b	Significant methodological deficiencies
3c	Unsuitable test system
4	**Not assignable**
4a	Abstract
4b	Secondary literature
4c	Original reference not yet available
4d	Original reference not yet translated
4e	Documentation insufficient for assessment